

Butanedioic acid, 2,2,3,3-tetrafluoro-  
377-38-8 | DTXSID8059928

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $7.68 \times 10^{-13}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $2.65 \times 10^{-1}$

**Confidence level:**  $5.73 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Trifluoro(trifluoromethoxy)ethylene

**Measured:**  $3.58 \times 10^{-12}$

**Predicted:**  $3.22 \times 10^{-12}$

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Acetic acid, trifluoro-

**Measured:**  $1.20 \times 10^{-13}$

**Predicted:**  $1.81 \times 10^{-13}$

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Acetic acid, trifluoro-, methyl ester

**Measured:**  $5.20 \times 10^{-14}$

**Predicted:**  $5.42 \times 10^{-14}$

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1,1,2,3,3,3-Hexafluoro-1-propene

**Measured:**  $2.20 \times 10^{-12}$

**Predicted:**  $2.03 \times 10^{-12}$

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Ethene, 1,1-dichloro-2,2-difluoro-

**Measured:**  $7.35 \times 10^{-12}$

**Predicted:**  $5.42 \times 10^{-12}$